INL/MIS-24-82303-Revision-0

Changing the World's Energy Future

TRISO fuel performance modeling in BISON

December 2024

Jacob Aaron Hirschhorn, Ryan Terrence Sweet

Idaho National Laboratory

INL is a U.S. Department of Energy National Laboratory operated by Battelle Energy Alliance, LLC

INL/MIS-24-82303-Revision-0

TRISO fuel performance modeling in BISON

Jacob Aaron Hirschhorn, Ryan Terrence Sweet

December 2024

Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

Prepared for the
U.S. Department of Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

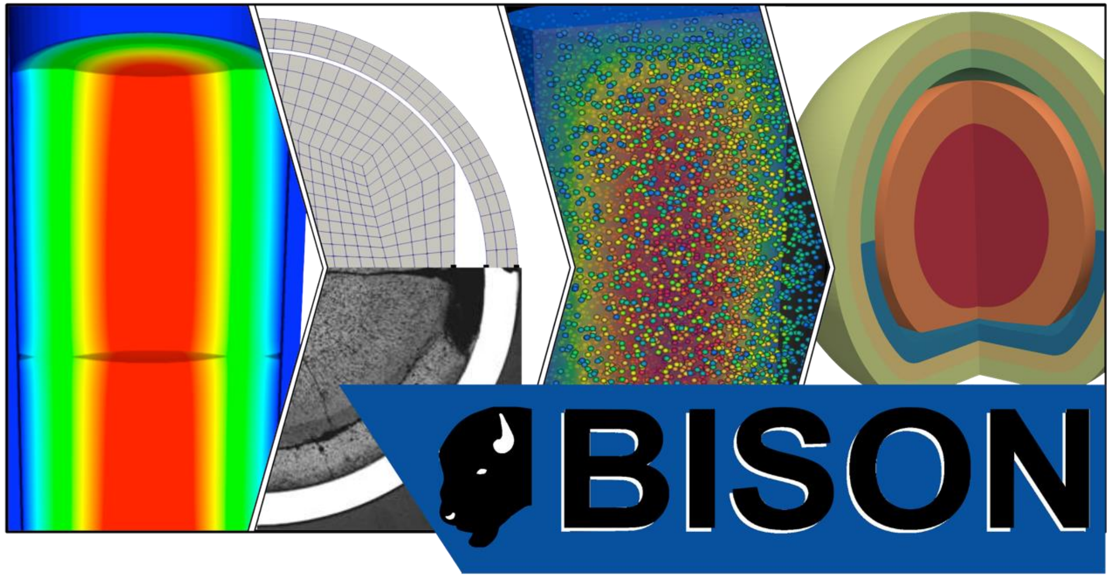
Jake Hirschhorn, Ph.D.
Computational Scientist, INL

Ryan Sweet, Ph.D.
Modeling and Simulation Engineer, INL

TRISO fuel performance modeling in BISON

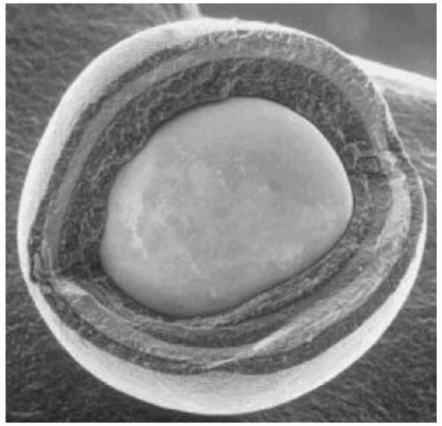
What is BISON?

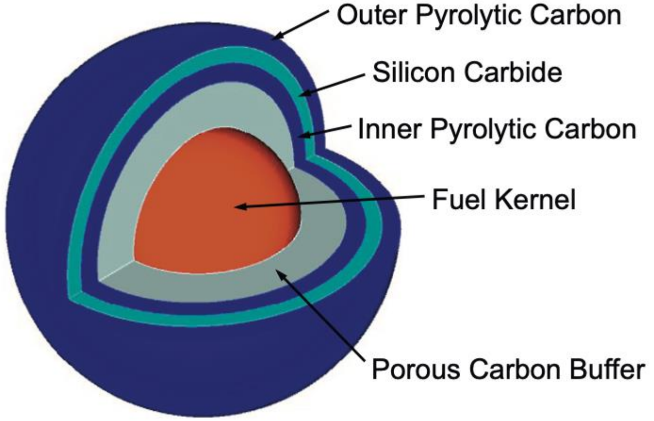
- BISON is a finite element-based nuclear fuel performance code
- Its development is currently funded by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program and a variety of other sources
- BISON is based on the MOOSE Framework
- BISON
  - Is free to use
  - Attracts diverse users and developers
  - Is used for engineering and research
  - Inherently considers multiphysics
  - Can couple to multiscale codes
  - Scales well from laptops to clusters
  - Features a flexible, modular design
  - Is under continuous development

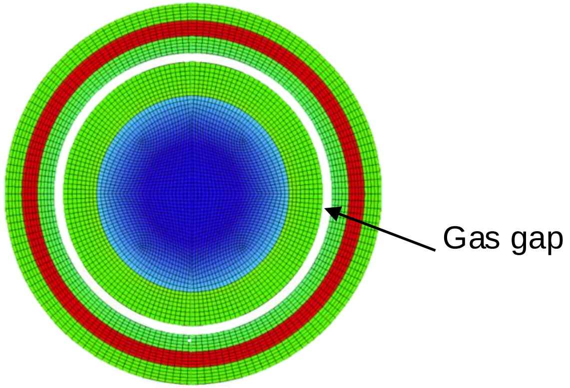


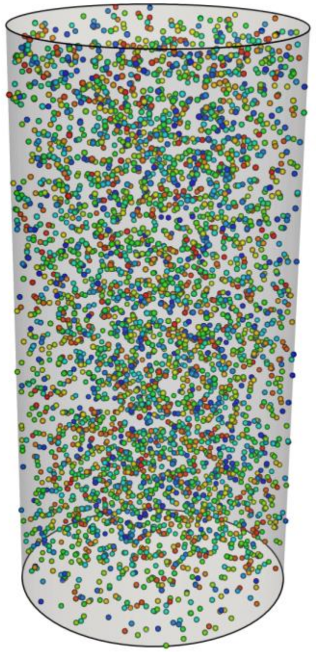
TRISO particle and compact anatomy

- TRISO fuel forms
  - Multi-layer, encapsulated fuel particles
  - Arranged within larger pebbles or pellets (compacts)
- Compact matrices
  - Graphite
  - SiC
  - Other carbonaceous materials



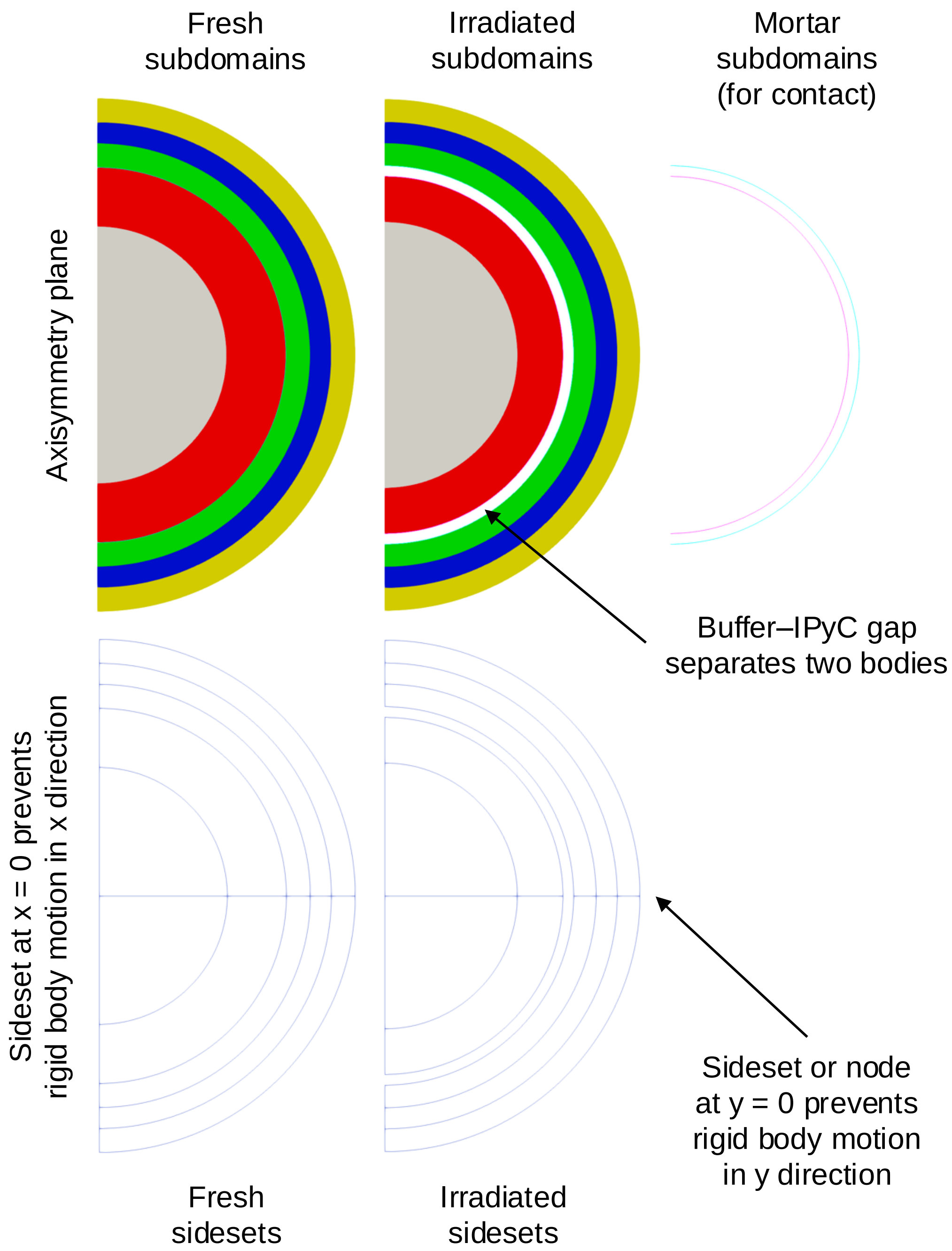






Adapted from works by Wen Jiang
J. Hales, et al., Journal of Nuclear Materials 443 (2013) 531-543.

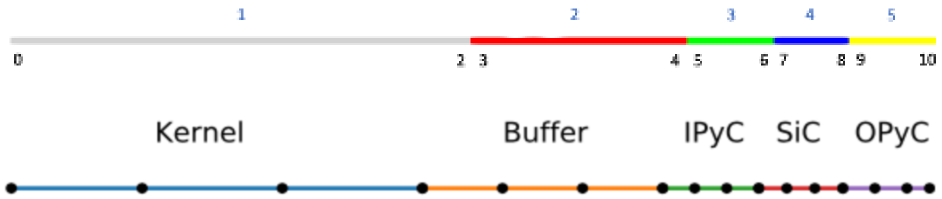
Goals of TRISO domain setup and discretization

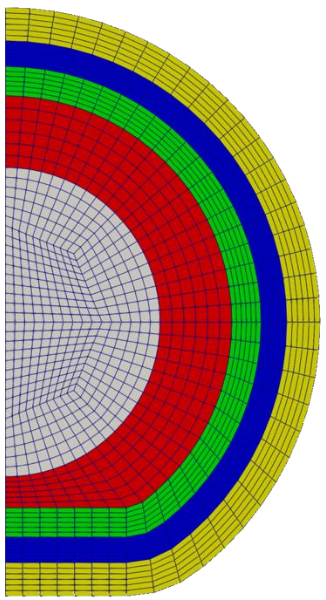


- Desirable features of computational domain setup
  - Accurate representation of the physical system geometry
  - Ability to setup a multibody problem
  - Ability to define different material properties on a subdomain basis
  - Ability to define continuous and discontinuous interfaces

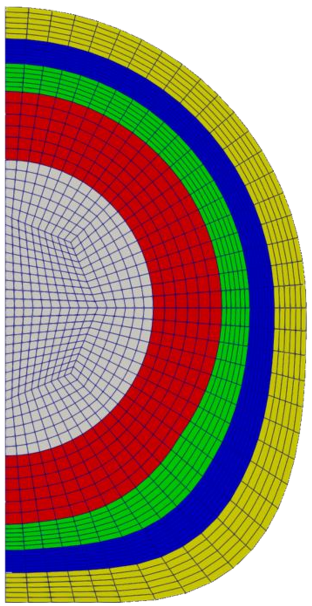
- Desirable features of discretization
  - Ability to apply boundary conditions
  - Flexibility in coordinate systems
  - Accuracy of solution
  - Efficiency of computation
  - Ability to take advantage of symmetry

Internal mesh generation is available for 1D, 2D, and 3D

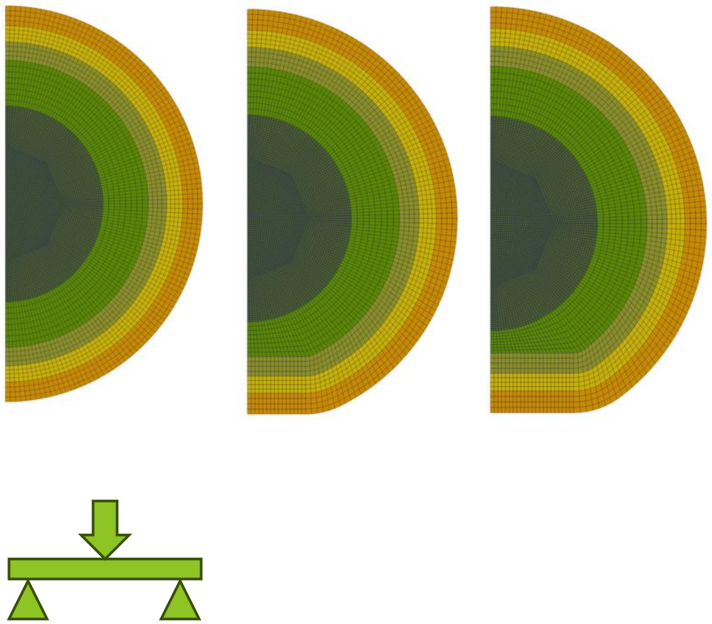


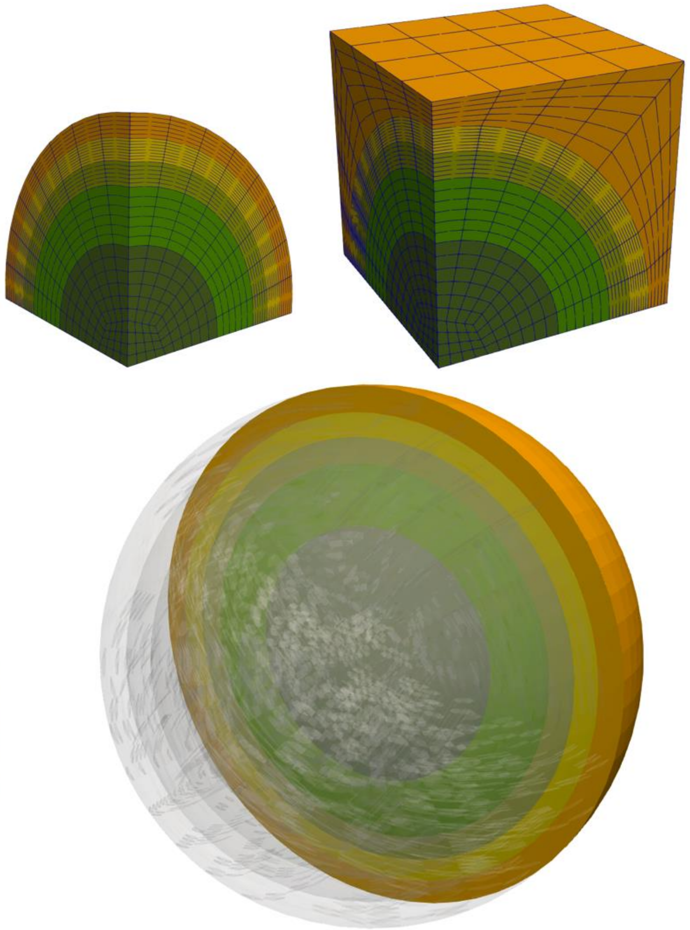


Original
“vary buffer”



Bezier
“vary outer”

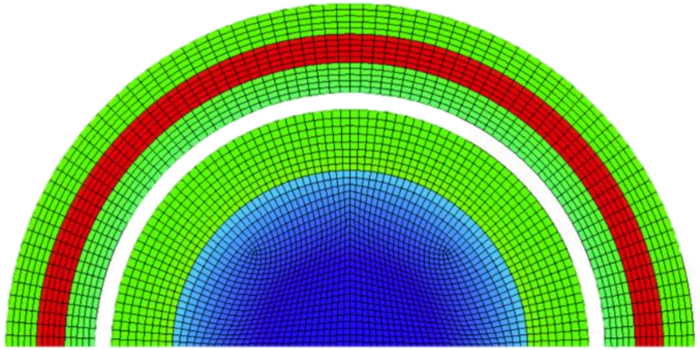




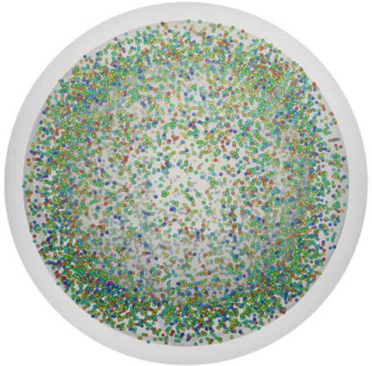
Adapted from works by Wen Jiang and Jason Hales

The particles themselves serve as the first barrier to release of fission products (FPs)

- Radionuclides of interest typically include isotopes of Cs, Sr, Ag, Kr, Xe, I
- We can model FP production, transport, decay, and release

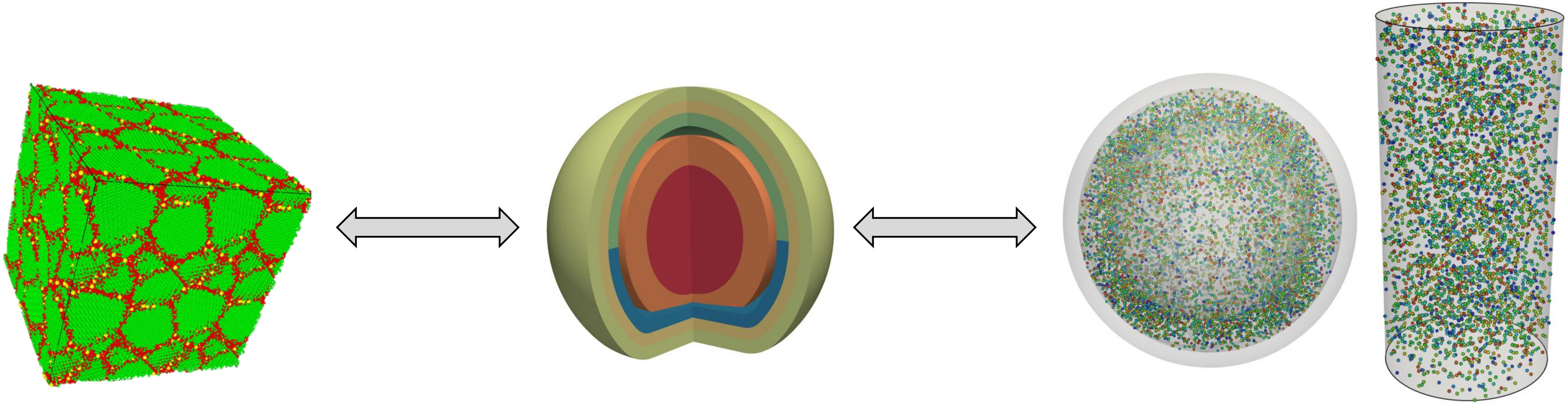


- Intra-layer and compact matrix diffusion are modeled as effective Fickian diffusion
- At the compact scale, particle source terms are weighted by failure probabilities



- The gas gap that forms at the buffer–IPyC interface during operation requires additional considerations
  - Thermal contact
  - Mechanical contact
  - Continuity or sorption mass transfer

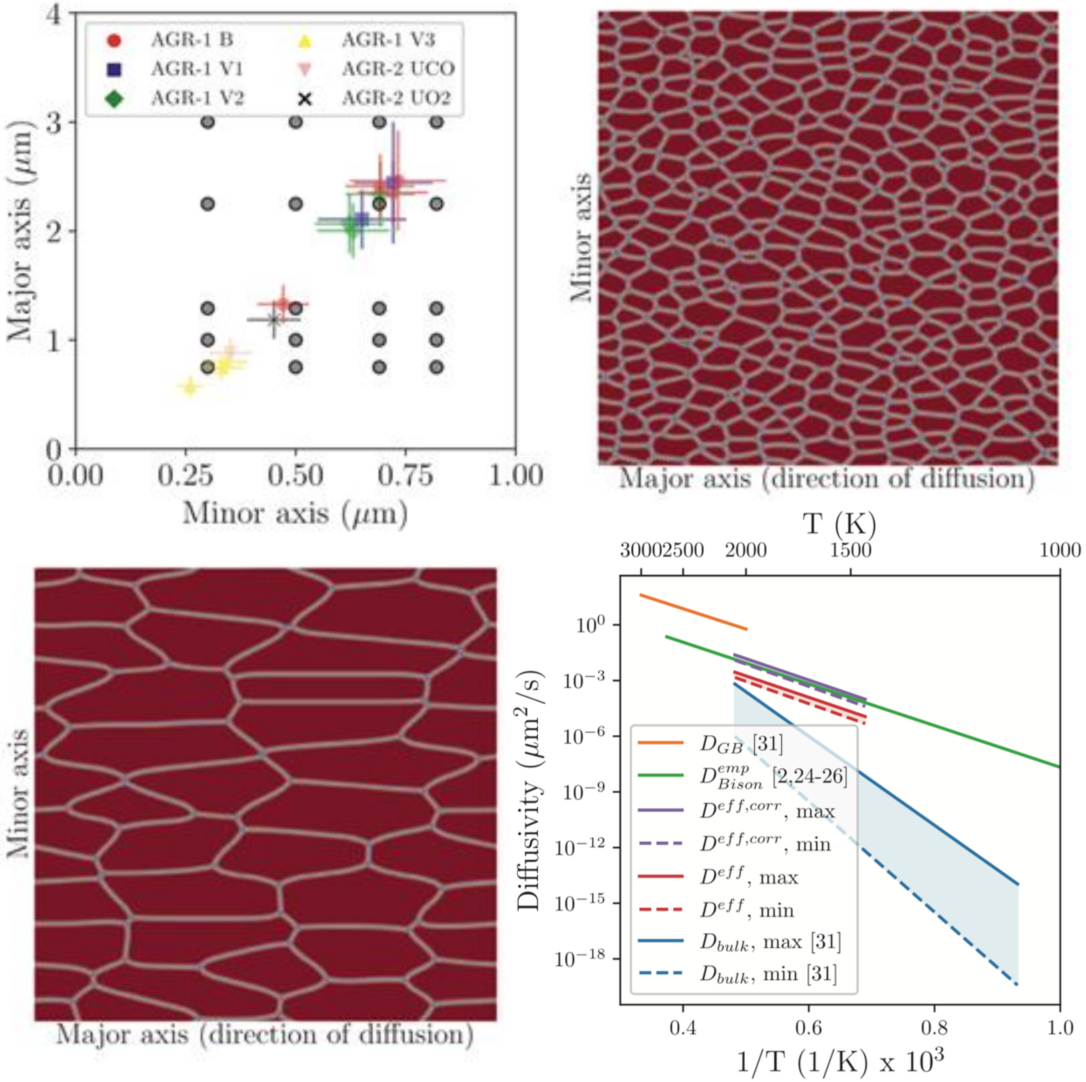
Multi-scale Transport Modeling Overview



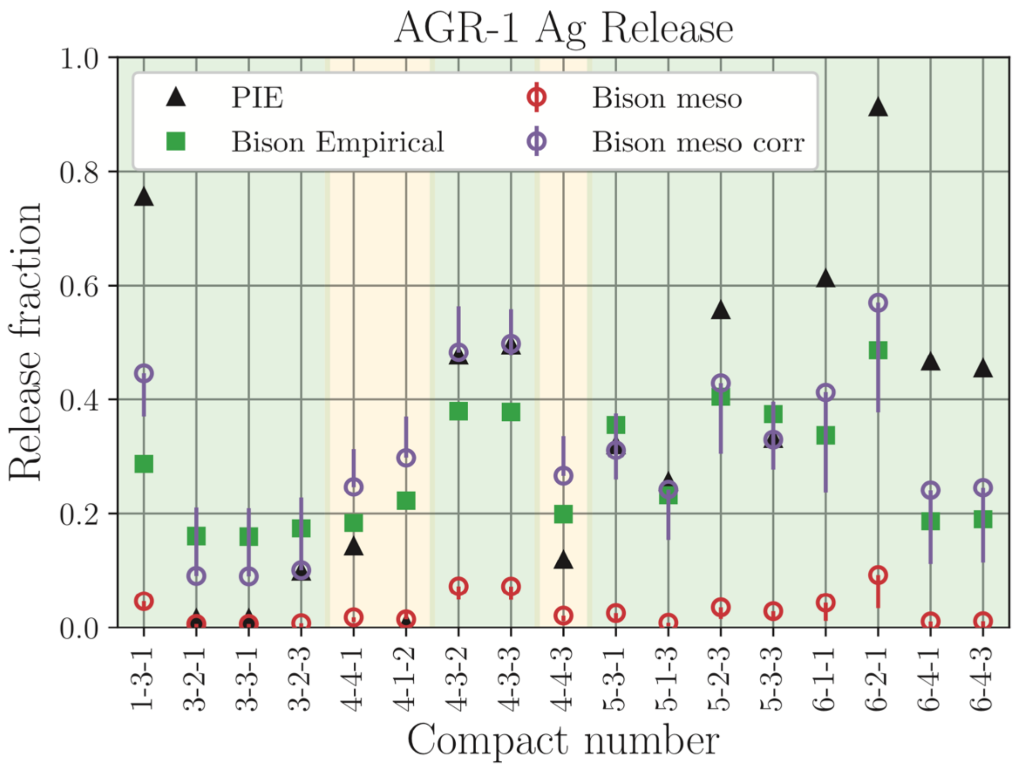
- Lower-length scale (LLS) modeling
  - Fission gas release model: Xe and Kr diffusivity in UCO
  - Fission product diffusivity: Pd penetration Ag diffusion in SiC
- Single TRISO particle modeling
  - Intralayer FP diffusion
  - Implicit sorption gap mass transfer
- Pebble and compact modeling
  - FP diffusion through matrix

Adapted from works by Wen Jiang

The BISON Team Works Closely with the MARMOT Team, Leveraging LLS Data to Improve Engineering Scale Models

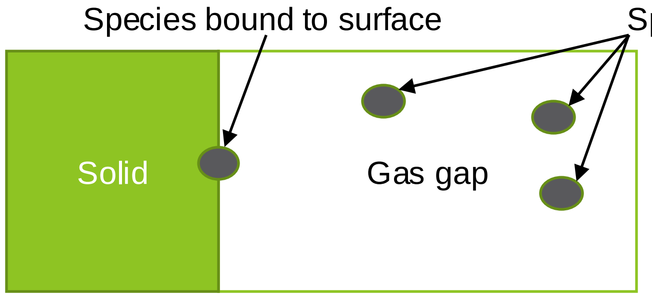


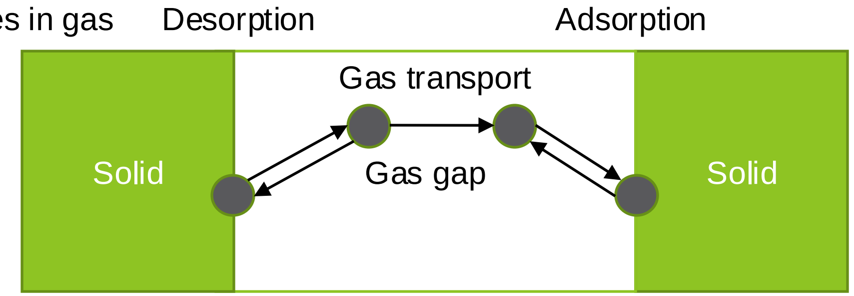
- Example: SiC microstructural data and models used to improve diffusivities



P-C. Simon, et al., Journal of Nuclear Materials 563 (2022) 153669.

Overview of Sorption Mass Transfer





- FP partial pressures at each surface are described by sorption isotherm data

$$P = \exp\left[\left(A + \frac{B}{T}\right) + \left(D - 1 + \frac{E}{T}\right)(d_1 - d_2 T)\right] c + \exp\left(A + \frac{B}{T}\right) c^{\left(D + \frac{E}{T}\right)}$$

(Henrian) (Freundlich)

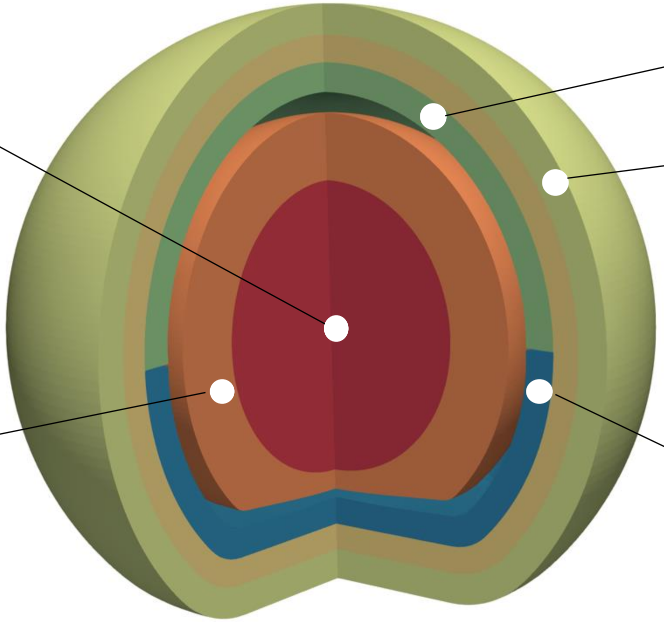
- Integral flux preservation is given by $\int_{\Omega_1} \boldsymbol{J_1} \cdot \boldsymbol{n_1} d\Omega_1 + \int_{\Omega_2} \boldsymbol{J_2} \cdot \boldsymbol{n_2} d\Omega_2 = 0$
- Assume
  - Partial pressure is homogeneous in the gap (equal at both surfaces)
  - Mass transfer across the unmeshed gap is instantaneous (implicit sorption assumption)
  - Engineering scale properties represent surface conditions (i.e., density)

Parameter	Description
P	Partial pressure
c	Concentration
T	Temperature
A	Sorption constants
B	
D	
E	
d_1	
d_2	
J	Mass flux
n	Outward unit normal
Ω	Surface area

Overview of BISON TRISO models

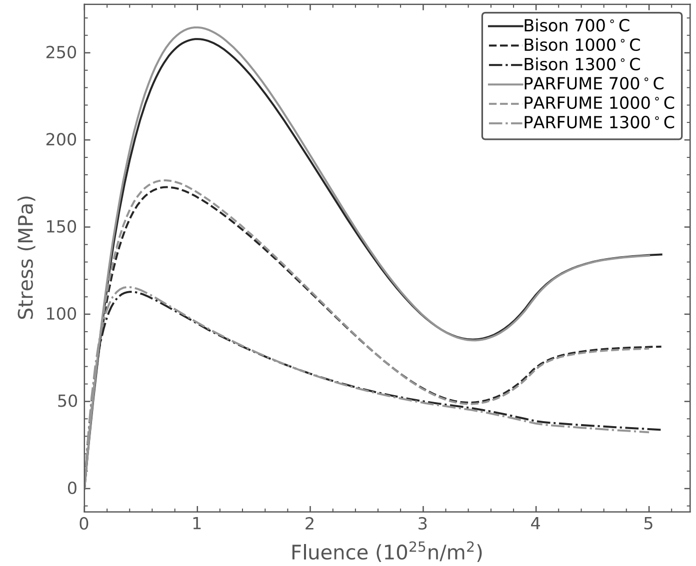
Kernel
Thermal
Burnup
Elasticity Tensor
Volumetric Swelling
Thermal Expansion
Fission Gas Release

Buffer
Thermal
Elasticity Tensor
Creep
Thermal Expansion
IIDC

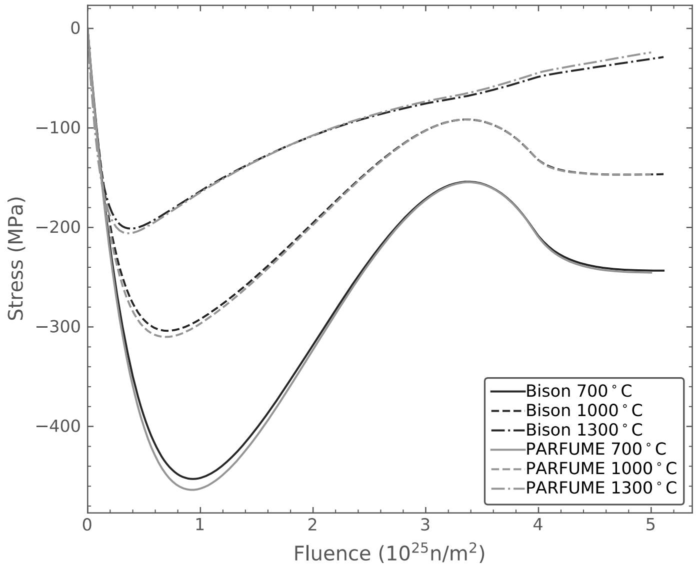


IPyC and OPyC
Thermal Expansion
Elasticity Tensor
Creep
IIDC

SiC
Elasticity Tensor
Thermal Expansion



Tangential stress in IPyC



Tangential stress in SiC

Adapted from works by Wen Jiang

The goals for modeling TRISO fuel performance, continued

- NRC provides guidance for nuclear power plants in 10 CFR Part 50 (primarily for monolithic LWR technology)

- Additional guidance SMRs and non-LWRs is given in NUREG-0800, NUREG-2246, and other topical reports

Specification	General Purpose(s)
Functional requirements	Maintain geometry, cooling, containment, and reloading capabilities
Operational requirements	Dictate power level, duty cycle, and requirements for performance during normal and off-normal operation (qualitative)
Fuel design criteria	Establish reactor- and fuel-specific specifications to ensure the above are met (quantitative)

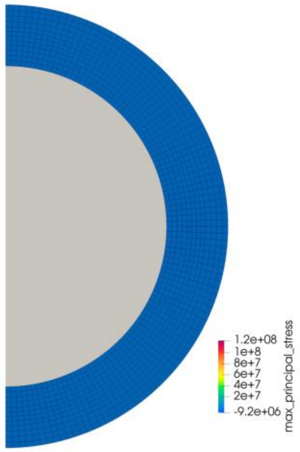
- General underlying goals include
  - Providing reactivity control
  - Maintaining cooling
  - Providing for fuel handling and storage
  - Enforcing quality standards
  - Containing radioactive nuclides
  - Recordkeeping

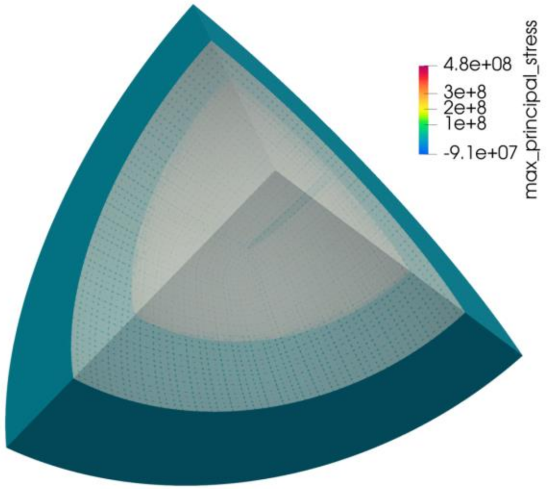
- Both intact and failed particles release fission products

- We need to calculate
  - How much radioactivity is released from each
  - The probability of particle failure

To Meet These Goals, We Need to Understand TRISO Behavior

- Three major categories
  - Deformation behaviors
  - Fission product (FP) transport
  - Failure behaviors
- TRISO particle behaviors
  - Kernel: volumetric swelling, burnup, thermal expansion, fission gas release
  - Fuel types: UCO, UO_2, and UN
  - Buffer and PyC: thermal expansion, irradiation-induced dimensional change (IIDC), irradiation creep
  - SiC: elasticity and thermal expansion
  - All: fission product production, transport, and release
- Compact/pebble behaviors
  - Graphite thermomechanical behaviors
  - FP transport through matrix



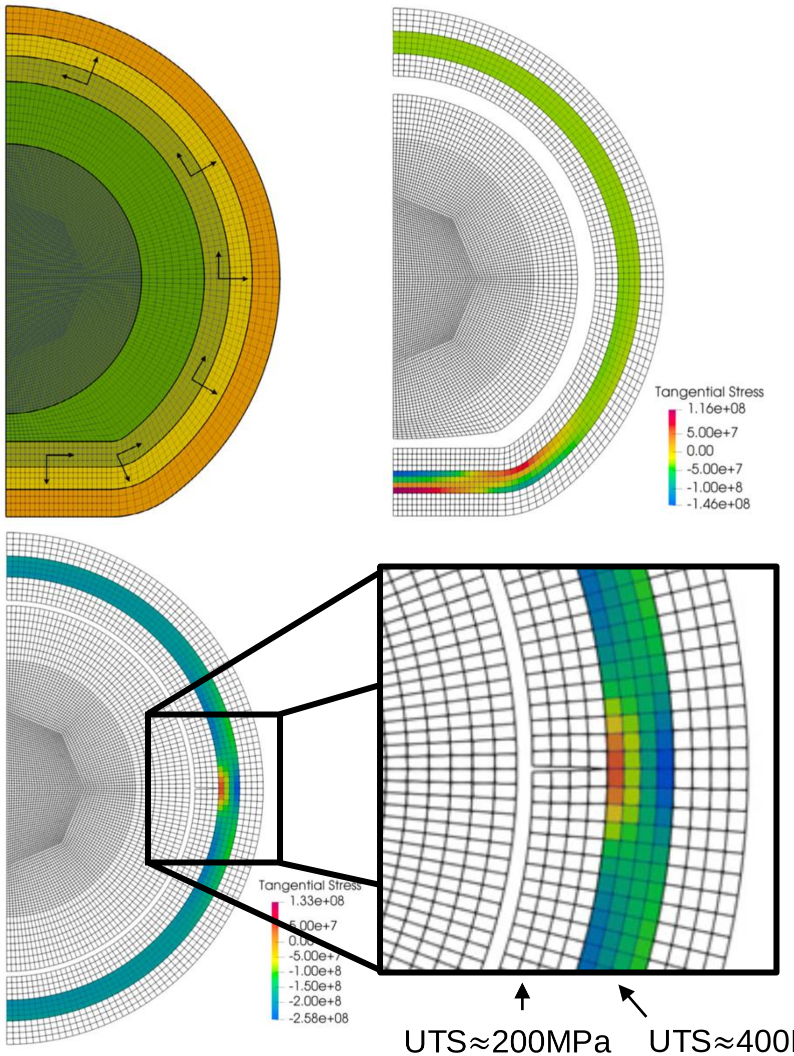


Adapted from works by Wen Jiang

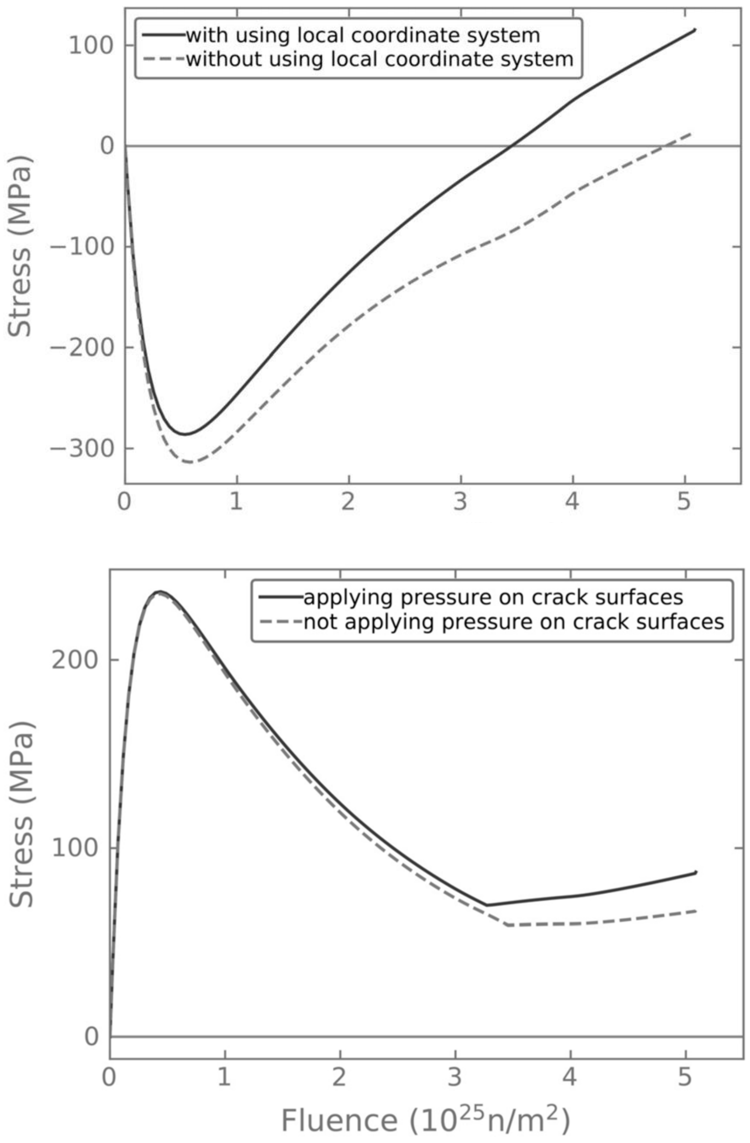
- TRISO particle failure modes
  - Pressure vessel failure (including asphericity)
  - Irradiation-induced PyC cracking
  - Debonding
  - Kernel migration
  - Palladium penetration
  - SiC thinning
- TRISO statistical failure analyses:
  - Monte Carlo
  - Direct integration
  - Variance reduction (importance sampling, subset simulation, etc.)

Additional models with inputs to failure calculations

- Asphericity, using local material coordinates to account for anisotropy
- IPyC cracking
  - Cracks are meshed using XFEM
  - Plenum pressure is applied to crack surfaces
- Debonding
  - Modeled using the cohesive zone method
  - Phase-field fracture and mortar methods are also available

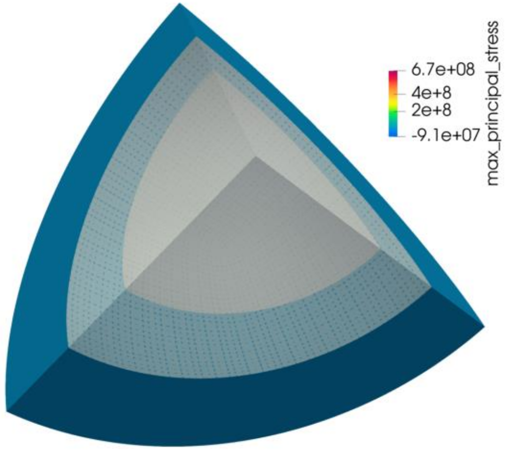


UTS≈200MPa UTS≈400MPa

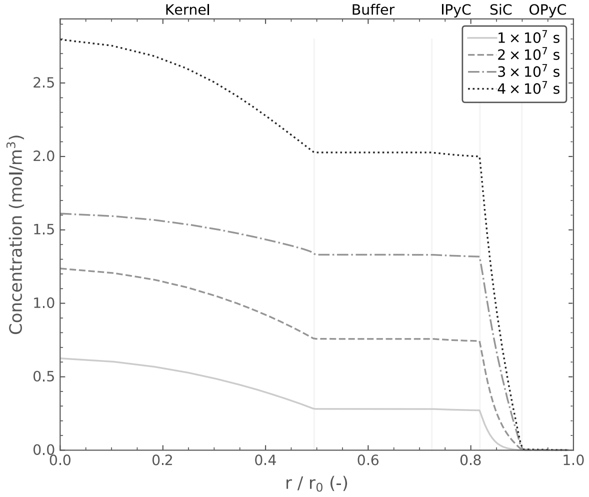


W. Jiang, et al., Journal of Nuclear Materials 562 (2022) 153585.

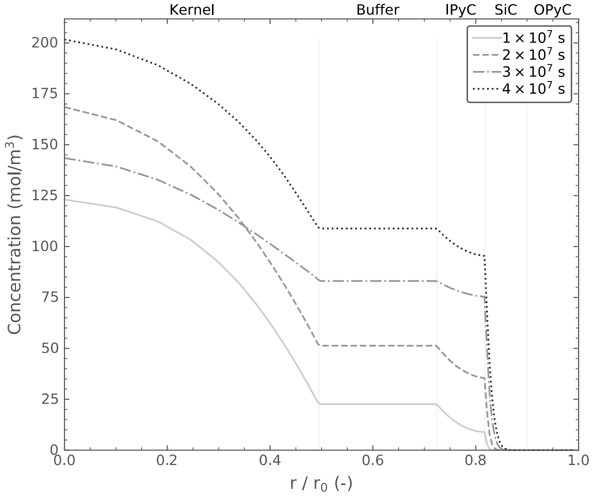
Species Diffusion in Intact and Failed Single Particles



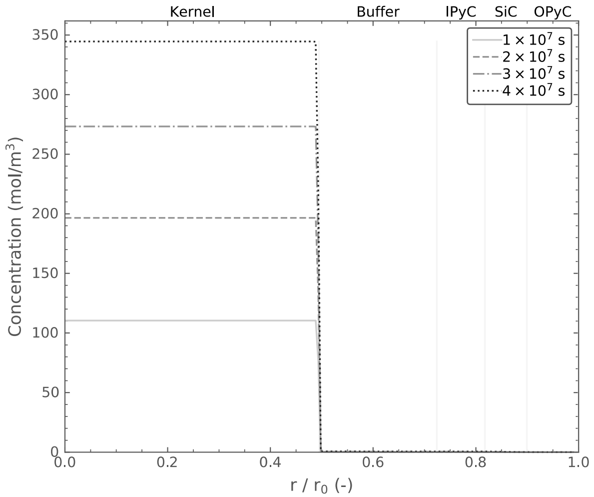
Intact



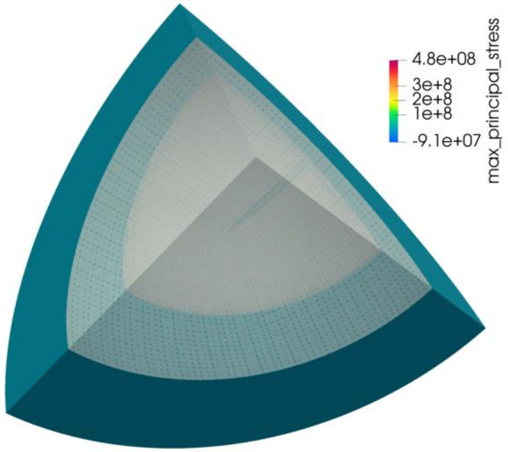
Silver



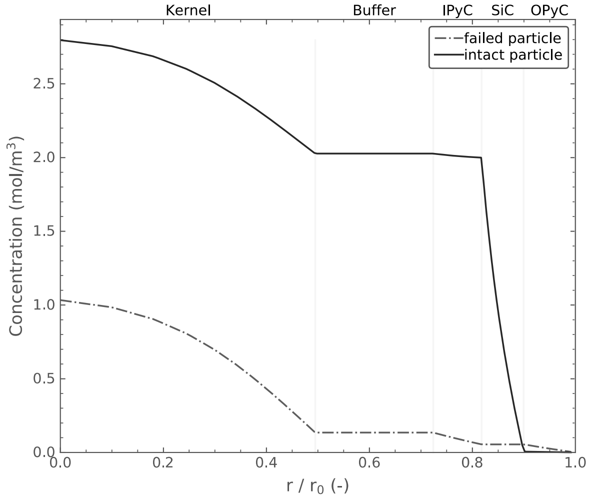
Cesium

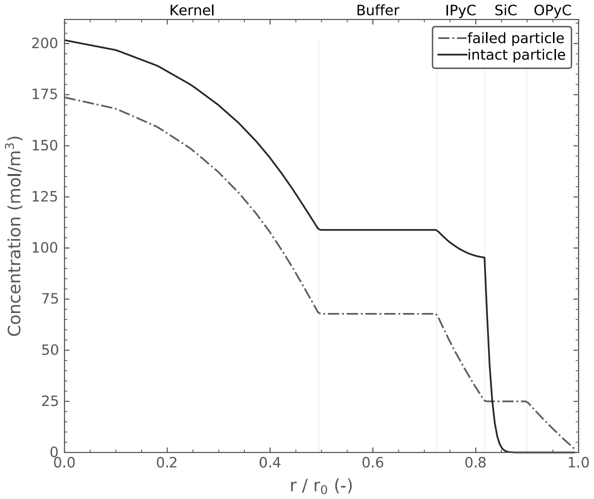


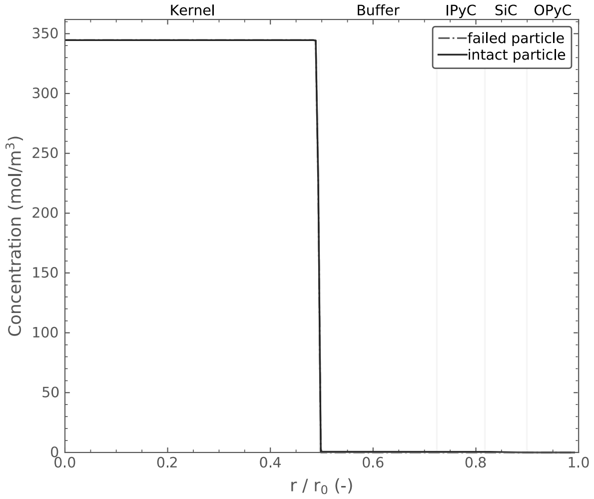
Strontium



Failed

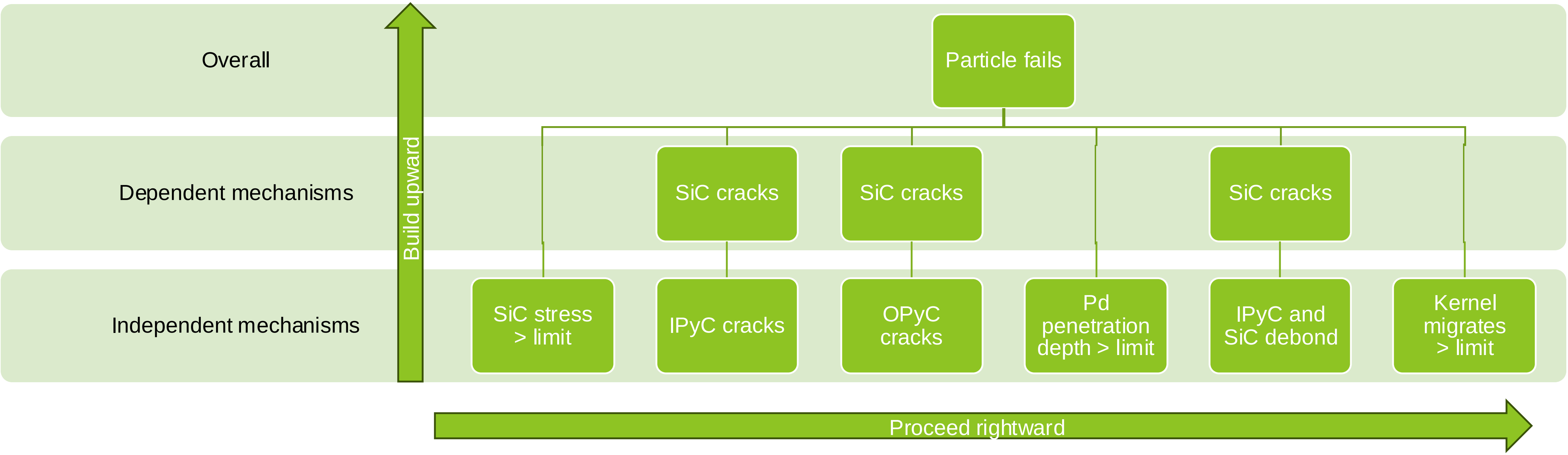






Adapted from works by Wen Jiang

Failure Mode Evaluations and Decision Making

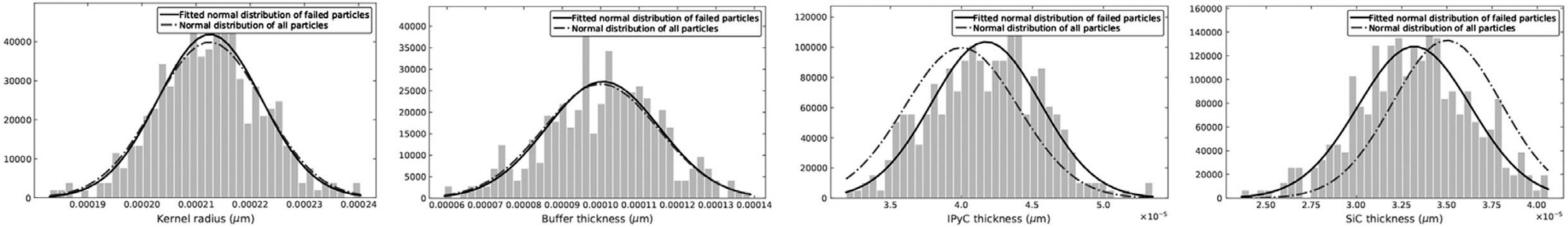


- SiC stress includes pressure vessel and asphericity effects

Overview of Failure Probability Calculations

- Variations in feedstock and fabrication conditions produce variations in particle by geometry, dimensions, and material properties
  - Layer thicknesses and densities
  - Particle asphericity, typically described by SiC aspect ratio or faceting
  - PyC anisotropy, typically described by Bacon anisotropy factor (BAF)

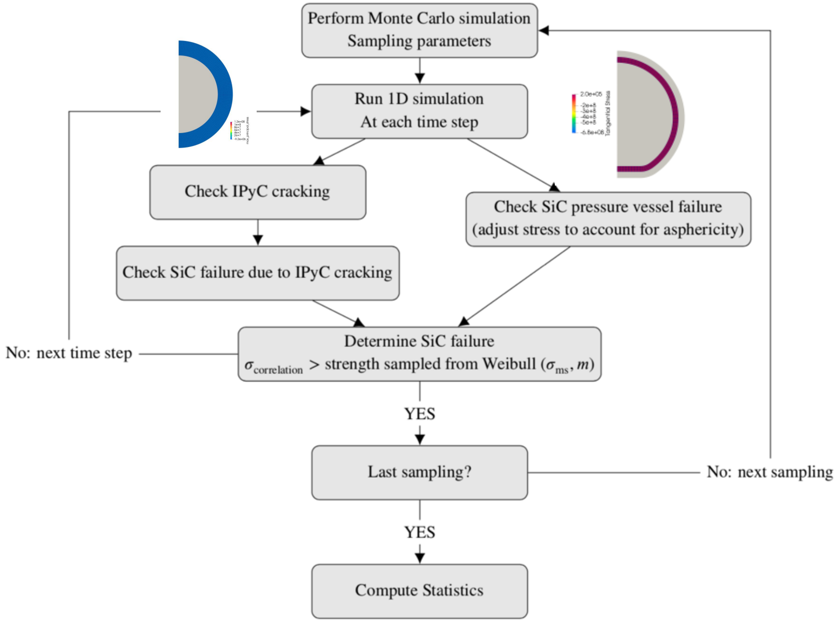
- Variations in these parameters impact fuel performance (i.e., likelihood of particle failure)

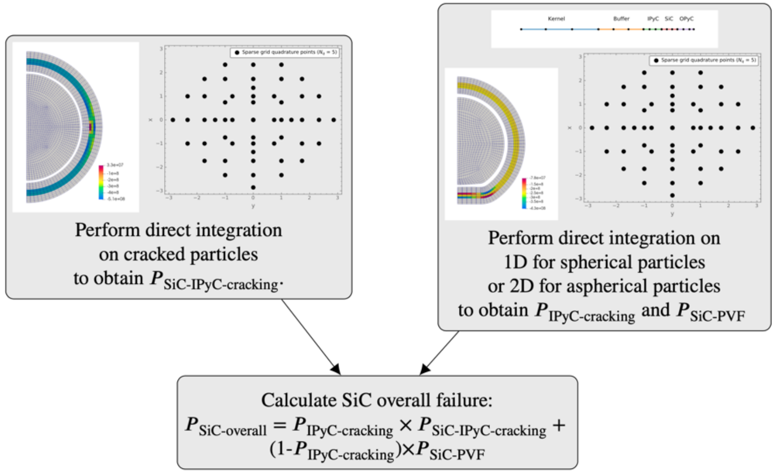


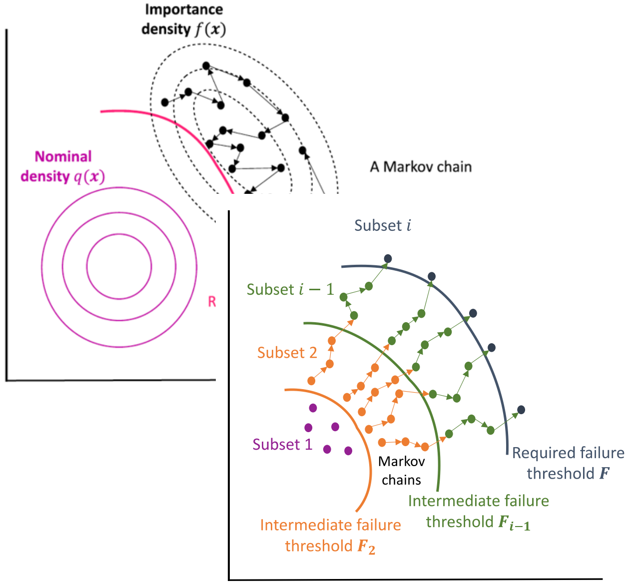
- The goal of failure probability calculations is to accurately predict the quantitative probability of failure of a population of particles having realistic variations in geometry, dimensions, and material properties

W. Jiang, et al., Journal of Nuclear Materials 548 (2021) 152795.

Failure Probability Calculation Methods



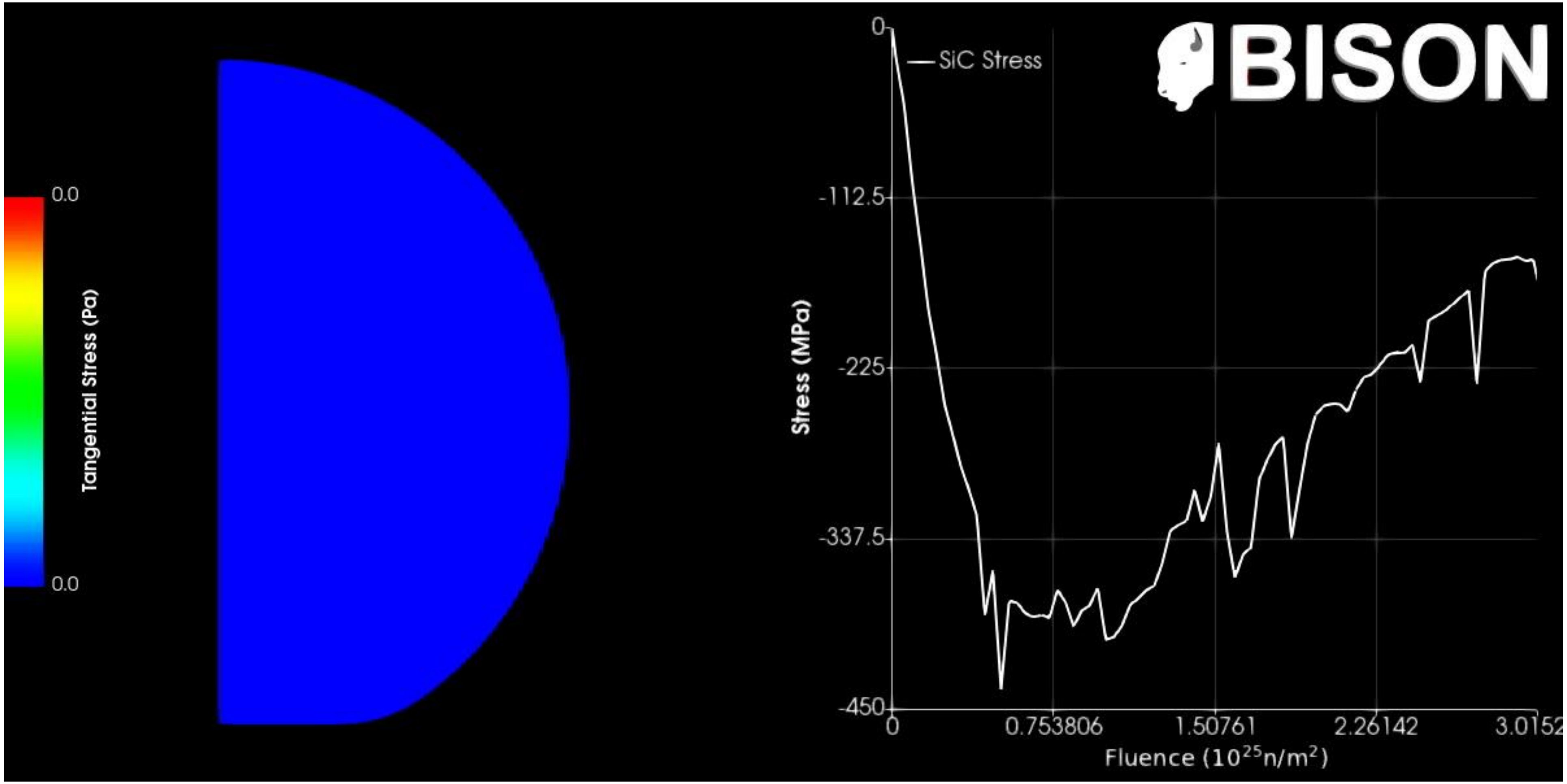




- Classical Monte Carlo approach
  - Most acceptable approach
  - Easy to expand for additional failure modes
  - Maximum of 100 million samples with parallel computing on HPC
- Direct Integration approach
  - Directly run 2D/3D TRISO simulations
  - Moderate computational cost, but still much less than the Monte Carlo approach
- Variance Reduction approach
  - Adaptive importance sampling and parallel subset simulation
  - Multi-fidelity TRISO failure modeling
  - Statistical failure characterization

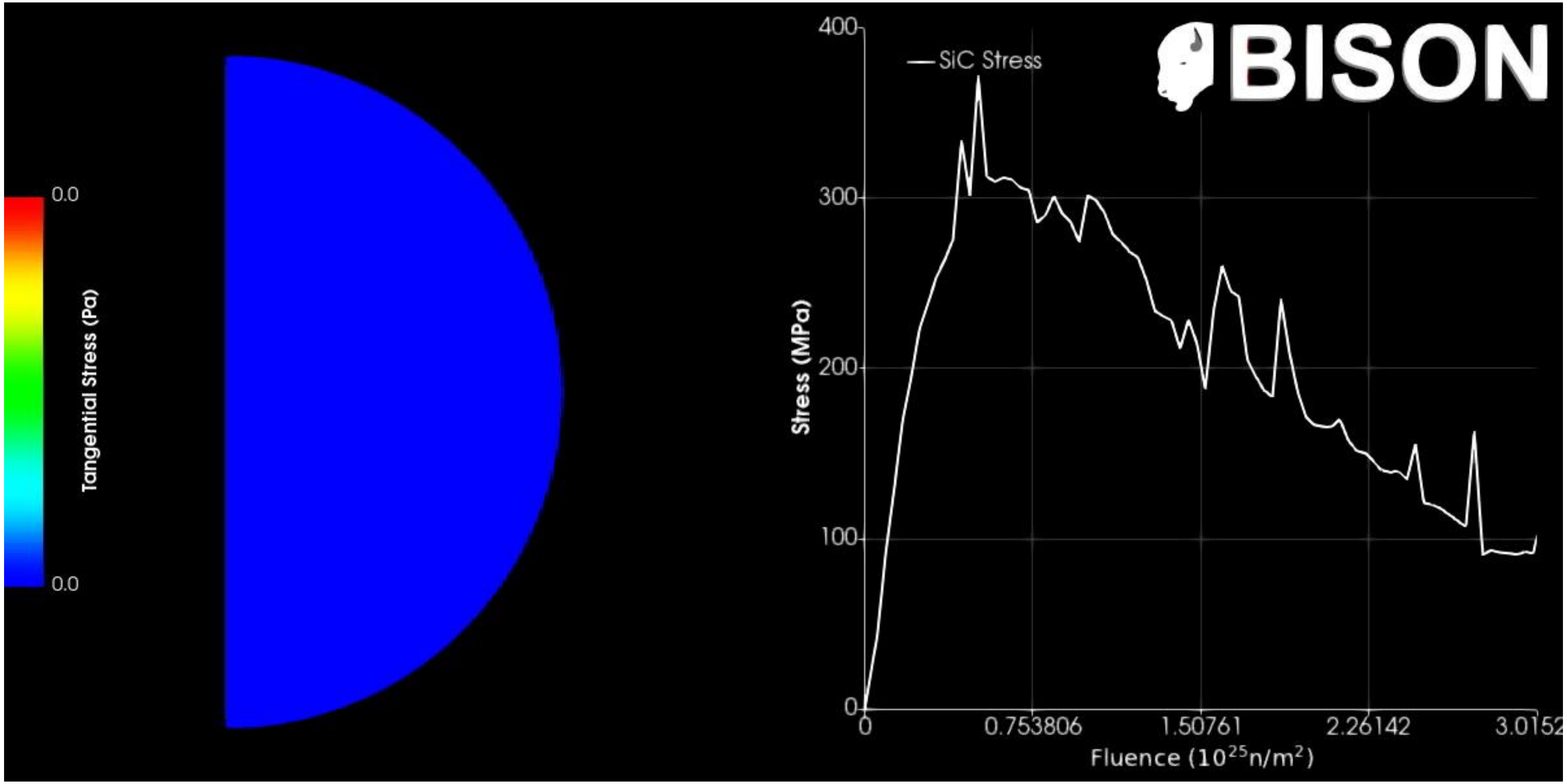
W. Jiang, et al., Journal of Nuclear Materials 548 (2021) 152795.
W. Jiang, et al., Journal of Nuclear Materials 562 (2022) 153585.
S. Dhulipala, et al., Journal of Nuclear Materials 563 (2022) 153604.

Pressure Vessel Failure with Asphericity Simulation



Adapted from works by Wen Jiang

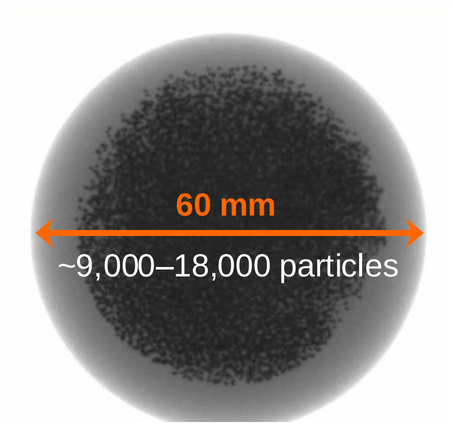
IPyC Cracking Simulation



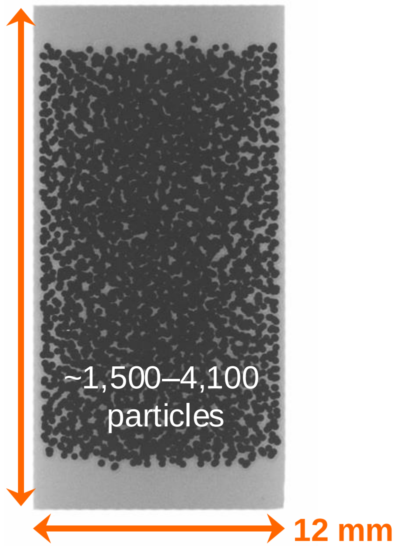
Adapted from works by Wen Jiang

Matrix Modeling

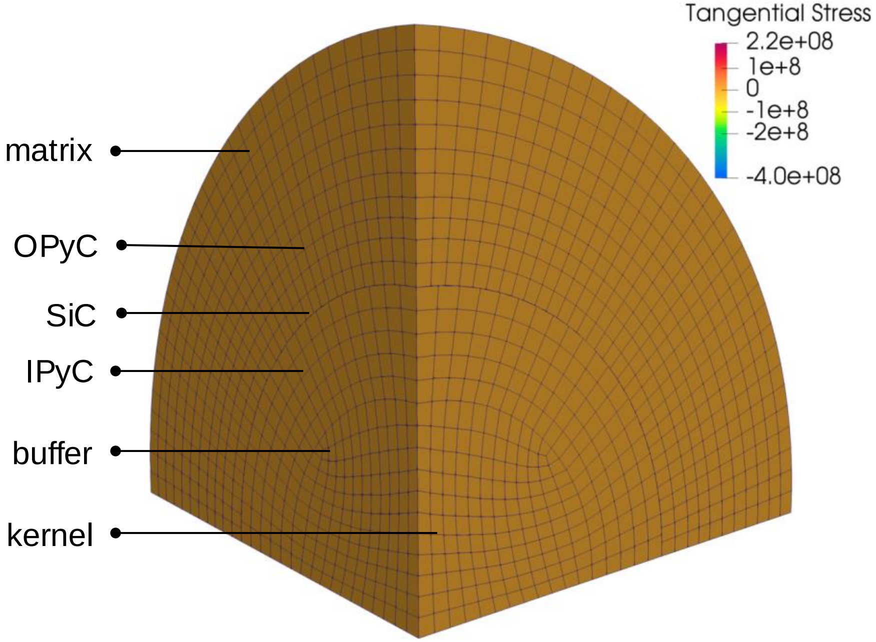
- Structural component, supporting fuel, coolant, and control rods
- Heat conduction path
- Affects moderation, reflection, and shielding



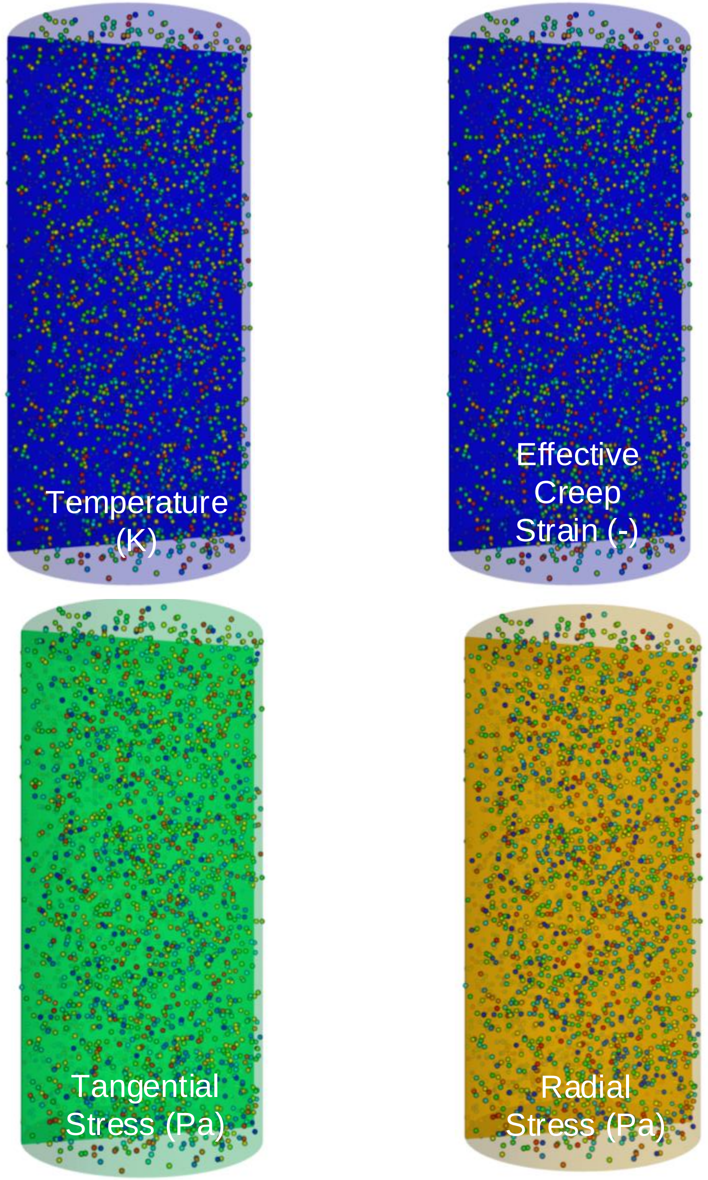
Spherical fuel elements



Cylindrical fuel elements

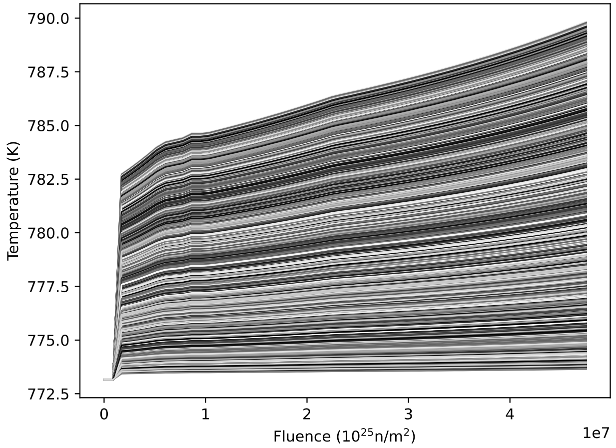


Tangential stress during irradiation for the particle-matrix debonding example (displacements are magnified 2X)

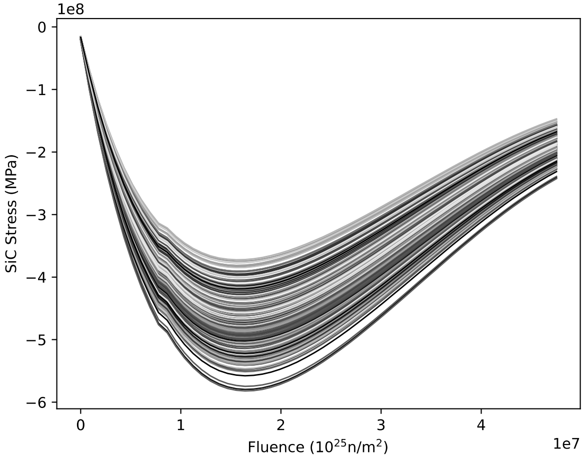


Adapted from works by Wen Jiang

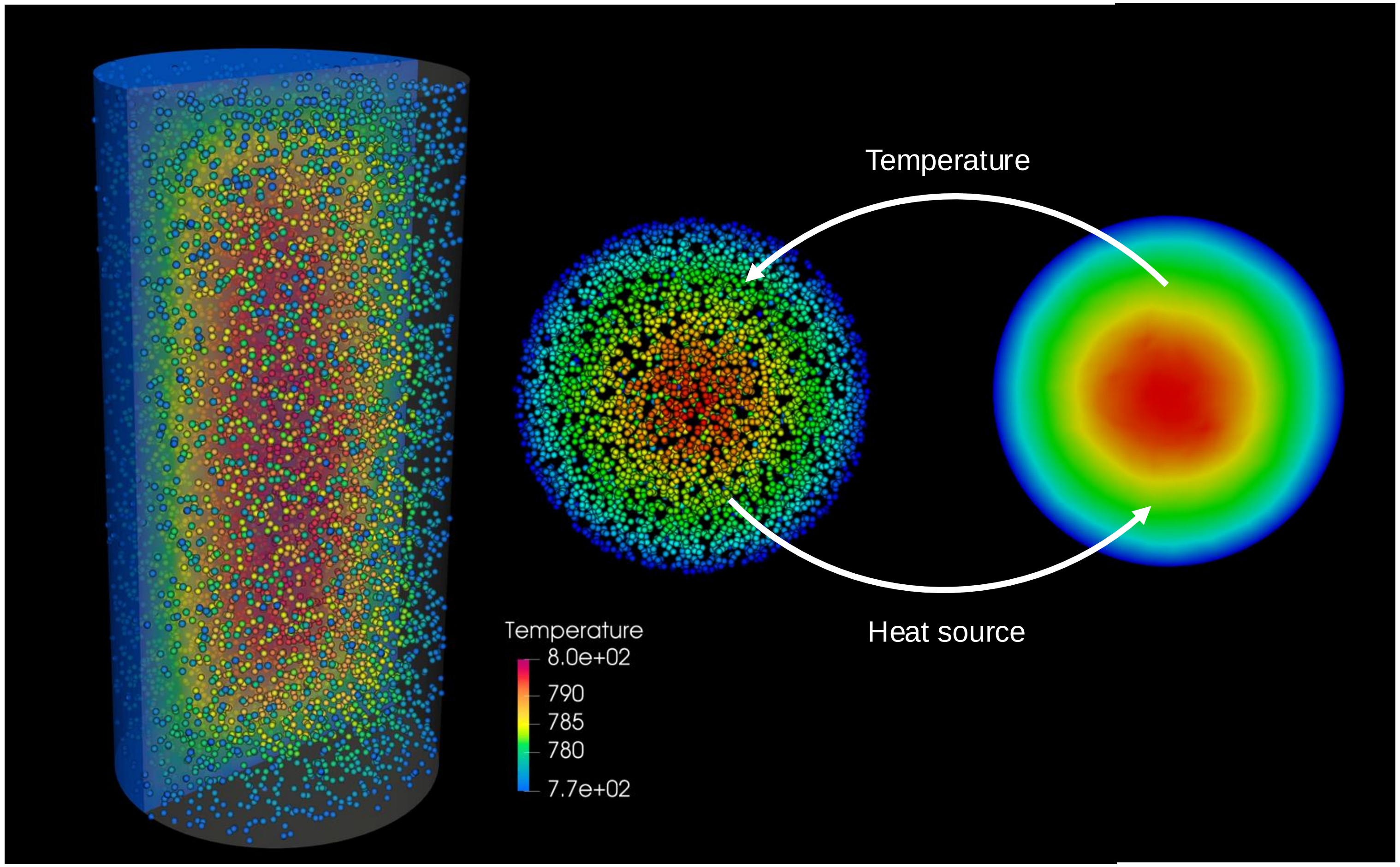
Point Source Method Allows Heat Transfer to Compact Matrix



Exterior temperature of all particles



SiC stress of all particles



Adapted from works by Wen Jiang

Idaho National Laboratory

Battelle Energy Alliance manages INL for the U.S. Department of Energy's Office of Nuclear Energy. INL is the nation's center for nuclear energy research and development, and also performs research in each of DOE's strategic goal areas: energy, national security, science and the environment.